X-ray Diffraction Study of β-Eucryptite $LiAlSiO_4$ at High Pressure and High Temperature *	X17B1

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The hexagonal aluminosilicate β-eucryptite ($LiAlSiO_4$) has remarkable thermal-expansion properties, with coefficients that are extremely anisotropic ($\alpha_a \approx 8.6\times10^{-6}$; $\alpha_c \approx$ -18.4$\times10^{-6}$ K^{-1}) and almost independent of temperature in the range 300-1400 K. In particular, the c axis shows negative thermal expansion over this temperature range ([1] and references therein). This material is also of continuing interest to earth scientists, due to its structural similarity to β-quartz (SiO_2), the major constituent in the Earths crust.

Energy-dispersive x-ray diffraction study was carried out on beta-eucryptite up to pressure of 2.5 GPa over the temperature range 300-1073 K. With increasing pressure, the diffraction peaks became broader at rate that was significantly faster than would be expected from the presence of microscopic deviatoric stress [2]. At 2.5 GPa, some low-intensity peaks were no longer identifiable. With increasing temperature at 2.5 GPa, diffraction peak widths showed little change up to 823 K, a behavior that is not expected if the broadening of peaks is caused by microscopic deviatoric stress. These observations indicate that this material was probably undergoing amorphization, even though the process was not completed. At 873 K, hexagonal beta-eucryptite transformed to rhombohedral structure, with all diffraction peaks that are very sharp. Upon cooling from 1073 K, the pressure was controlled, by manual adjustment of oil pressure, to be constant within 0.1 GPa of the desired values (1.95 GPa) at each temperature condition, and the data were collected at intervals of 50-100 K. These isobaric data reveal that rhombohedral eucryptite shows normal thermal-expansion behavior, with coefficients that increase with temperature for both a and c crystallographic axes.

References:

[1] Lichtenstein, et al. (1998) Phys. Rev. B 58: 6219-6223

[2] Weidner, et al. (1992) In Syono Y and Manghnani, MH (ed.) High-Pressure Research: Application to Earth and Planetary Sciences. AGU, Washington DC, Geophysics Monograph Series, Vol. 67, pp. 1317.

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